Science with 4th-Generation X-Ray Sources

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SSRL/SLAC

Workshop on Detectors for
Synchrotron Research
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SSRL

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What distinguishes a 4th-generation x-ray source? How is FEL radiation different from synchrotron radiation?

What exciting science will be done with 4th-generation x-ray sources?

What special detectors will be needed for this science?

Synchrotron radiation *vs.* FEL radiation

The difference is in the electron beam quality

Conventional synchrotron radiation
Electron brightness << diffraction limit of emitted radiation

Electromagnetic field effects on the electrons are not significant

Each electron radiates independently, not coherently with others

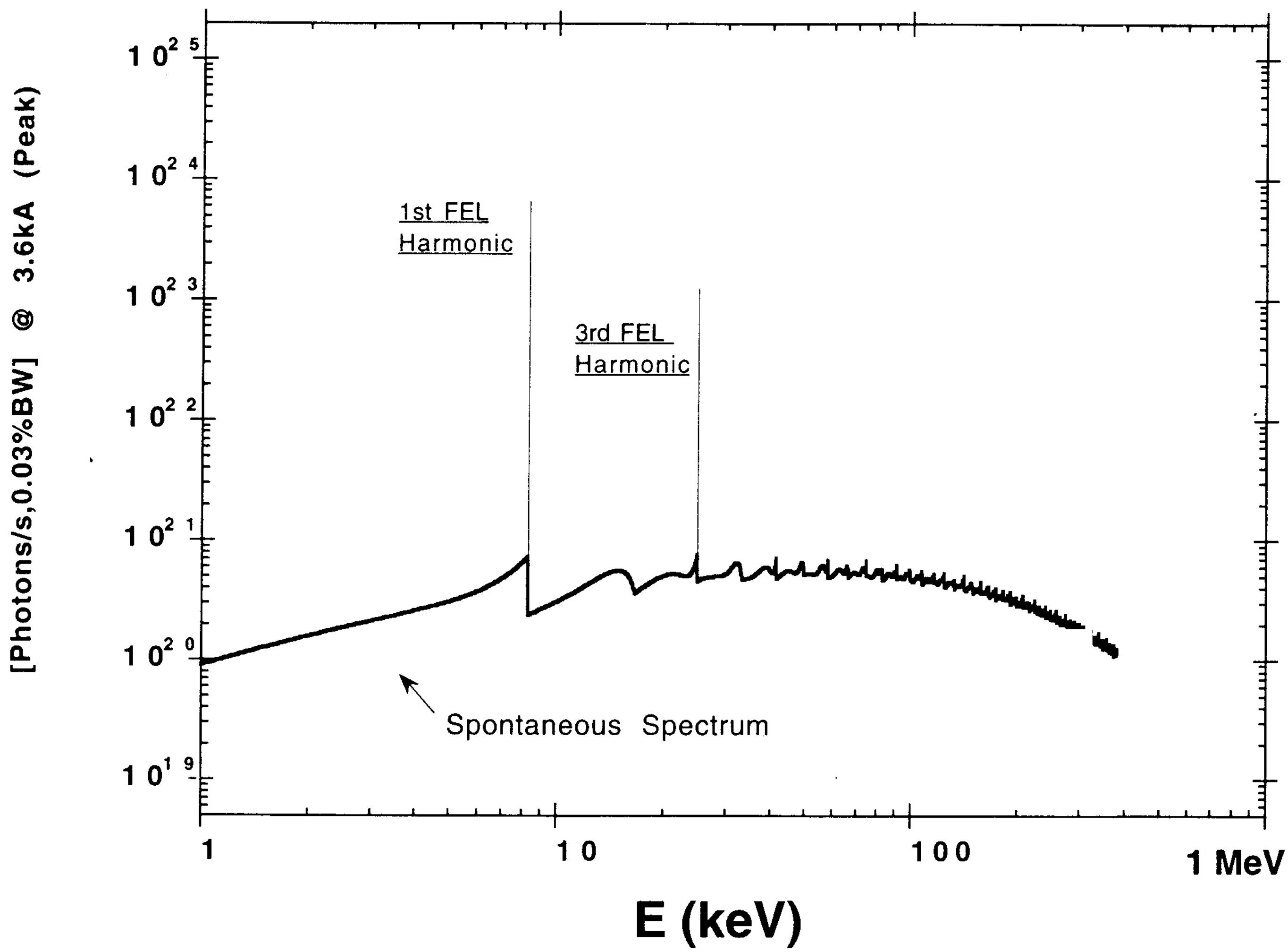
Free Electron Laser radiation
Electron brightness ~ diffraction limit of radiation

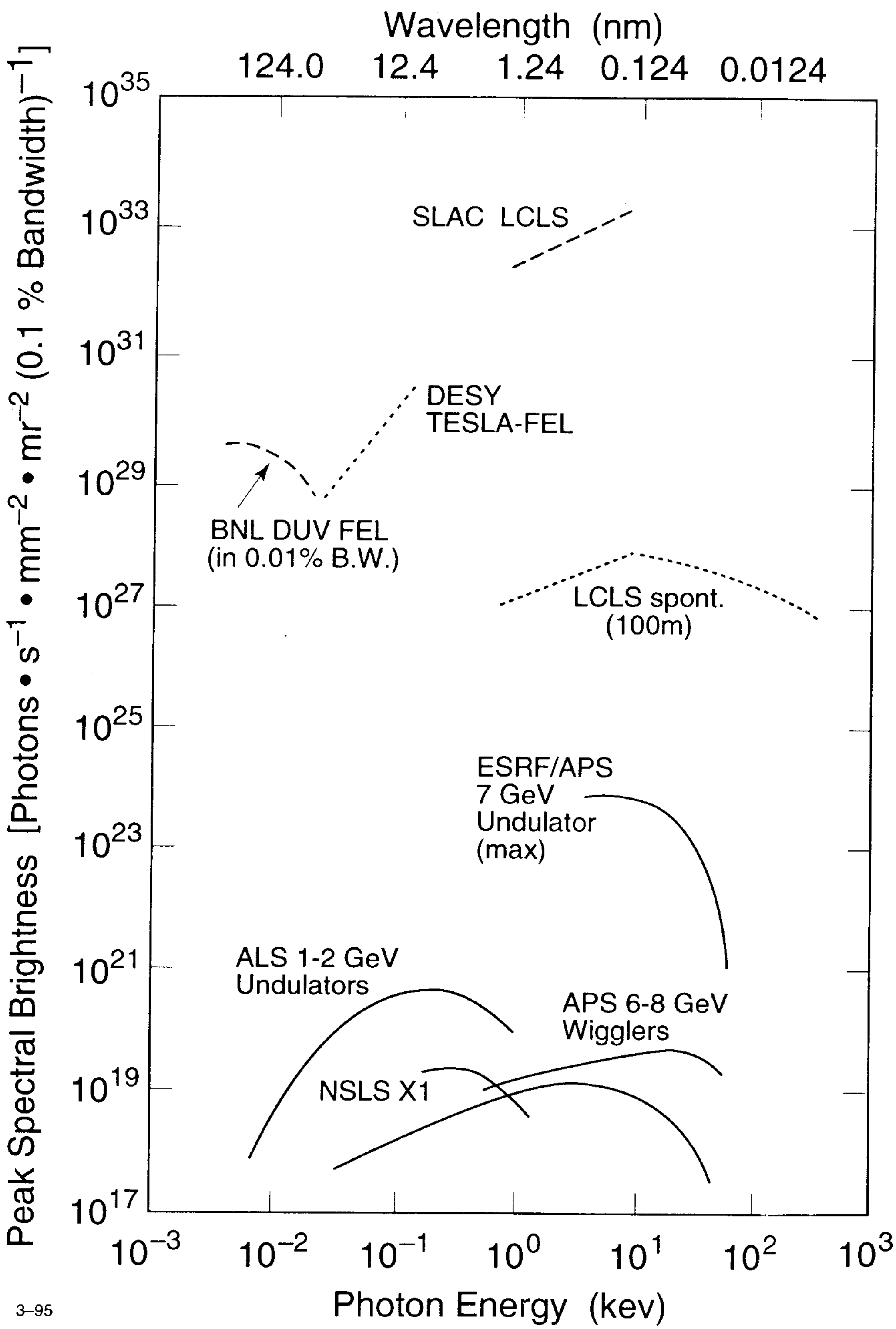
EM field can cause microbunching of electrons, on scale of radiation wavelength

Electrons radiate collectively, coherently

LCLS Peak Photon Flux Spectrum

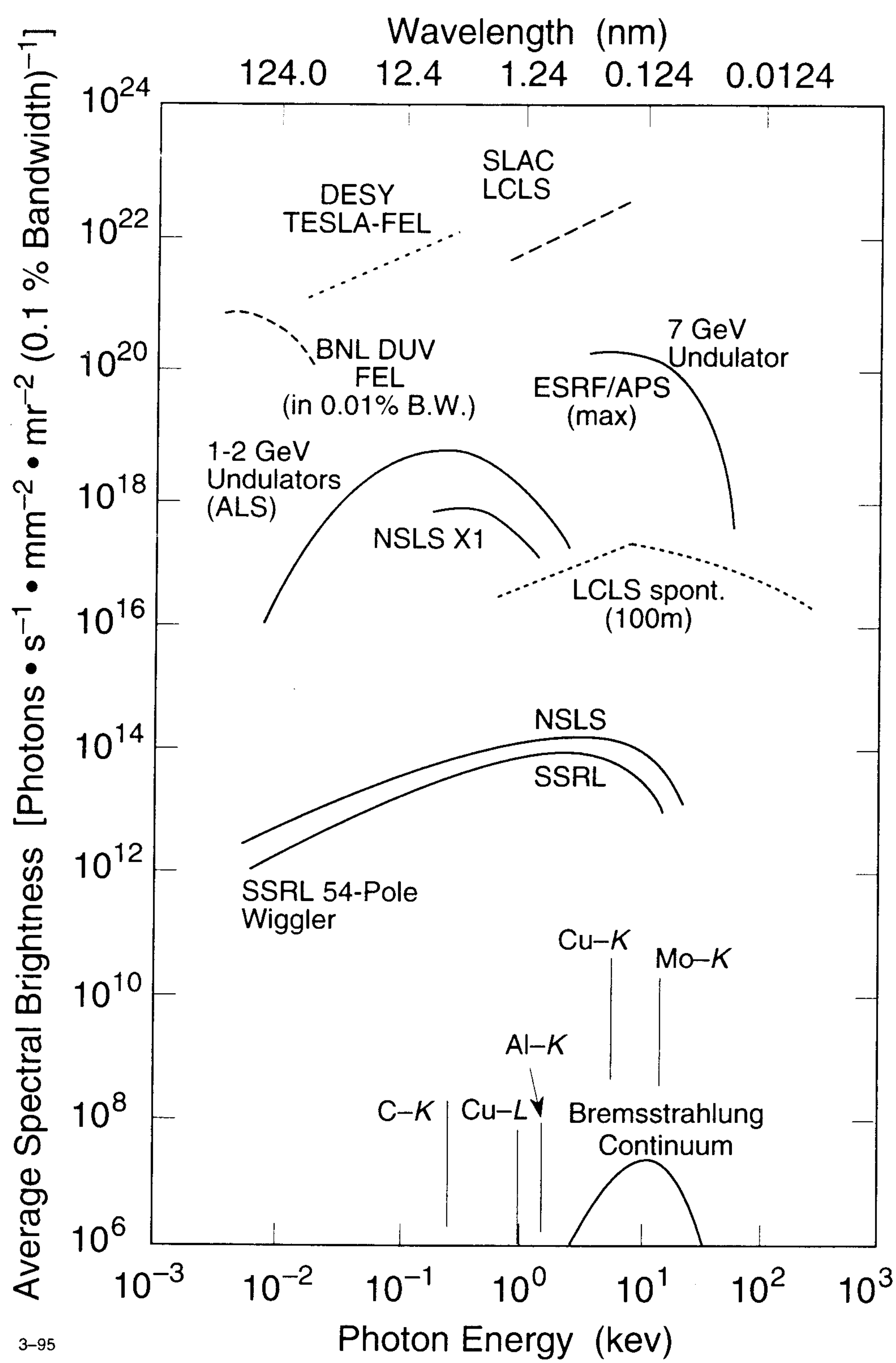
3300 periods, K=3.7, E=14.35 GeV, 120 Hz rep rate





Wavelength (nm)
124.0
12.4
1.24
0.124
0.0124
10^{35}
10^{33}
10^{31}
10^{29}
10^{27}
10^{25}
10^{23}
10^{21}
10^{19}
10^{17}
Peak Spectral Brightness [Photons • s^{-1} • mm^{-2} • mr^{-2} (0.1 % Bandwidth)$^{-1}$]
SLAC LCLS
DESY
TESLA-FEL
BNL DUV FEL
(in 0.01% B.W.)
LCLS spont.
(100m)
ESRF/APS
7 GeV
Undulator
(max)
ALS 1-2 GeV
Undulators
APS 6-8 GeV
Wigglers
NSLS X1
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Photon Energy (kev)

3–95


Wavelength (nm)
124.0
12.4
1.24
0.124
0.0124
Average Spectral Brightness [Photons • s^{-1} • mm^{-2} • mr^{-2} (0.1 % Bandwidth)$^{-1}$]
10^{24}
10^{22}
10^{20}
10^{18}
10^{16}
10^{14}
10^{12}
10^{10}
10^{8}
10^{6}
SLAC
LCLS
DESY
TESLA-FEL
BNL DUV
FEL
(in 0.01% B.W.)
7 GeV
Undulator
ESRF/APS
(max)
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Undulators
(ALS)
NSLS X1
LCLS spont.
(100m)
NSLS
SSRL
SSRL 54-Pole
Wiggler
Cu–*K*
Mo–*K*
Al–*K*
C–*K*
Cu–*L*
Bremsstrahlung
Continuum
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Photon Energy (kev)
3–95

Key features of X-Ray FEL Radiation

- Sub-picosecond pulse

  230 fs FWHM pulse with 1 fs structure

- Very high peak power and brightness

  More than 10^{12} photons/pulse

  Degeneracy factor greater than 10^{9}
  (APS undulator degen. factor is <1)

- Full spatial coherence

  A diffraction-limited x-ray source

Calculated Characteristics of the LCLS beam

FEL wavelength	1.5	Å
Bandwidth (δE/E)	0.002	
Pulse duration (FWHM)	233	fs
Pulse length (FWHM)	70	μm
Peak coherent power	9	GW
Energy/pulse	2.6	mJ (2 mJ = 2×10^{16} eV)
Peak coherent power density	2×10^{12}	W/mm^2
Peak brightness	1×10^{33}	flux/mm^2/mrad^2/0.1%BW
Coherent photons/pulse	2×10^{12}	
Coherent photons/second	2×10^{14}	
Degeneracy parameter	10^9	
Peak EM field (unfocussed)	3×10^{10}	V/m
Repetition rate	120	Hz
Average coherent power	0.3	W
Average brightness	2×10^{22}	flux/mm^2/mrad^2/0.1%BW
Transverse size of coherent radiation (FWHM)	80	μm
Divergence of coherent radiation (FWHM)	1	μrad
Peak power of spontaneous (wide spectrum) radiation	81	GW

FEL wavelength tuning range: 15-1.5 Å = 0.8-8 keV

Spontaneous radiation spectrum: 0.3-30 x FEL energy
(i.e., 2.4-240 keV for FEL energy of 8 keV)

Atomic Physics

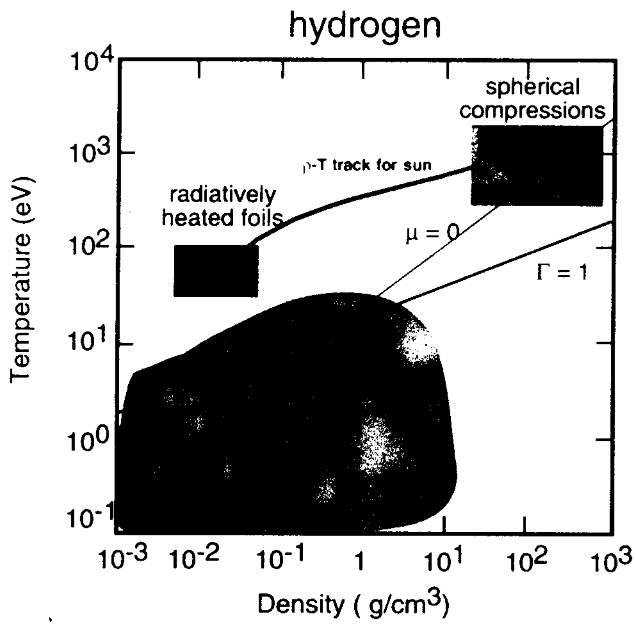
Atom interactions with x-ray FEL pulse are different from interactions with conventional lasers or weaker x-ray sources

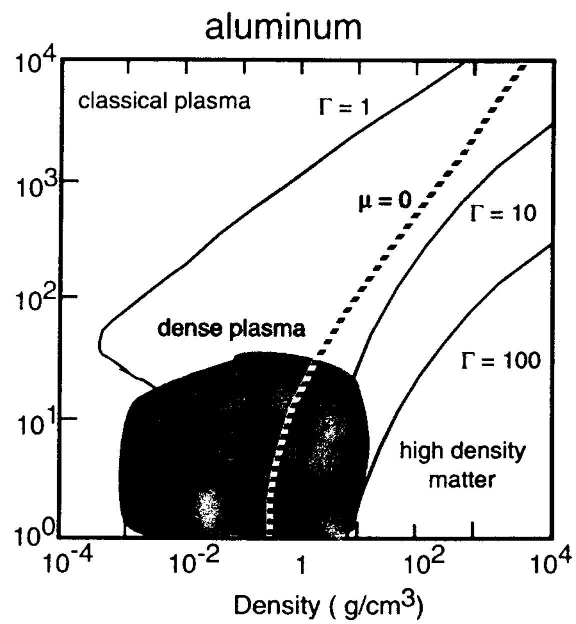
Studying LCLS-atom interactions will advance atomic physics and provide basis for understanding all other LCLS experiments

- Direct observation of multiple core hole formation (MCHF) in an atom
- Direct observation of multiphoton ionization of a K-shell electron (MPIK)
- Observation of giant coulomb explosions in atomic cluster (GCEC)
- Studies of radiation and possibly lasing from XFEL-excited matter
- Formation of highly excited laser plasmas

Studies of Warm Dense Matter

"...that part of the density-temperature phase space where the standard theories of condensed matter physics and/or plasma statistical physics are invalid."





Γ = ratio between electric and thermal potential energy
μ = chemical potential (atom interaction potential)

LCLS will be able, for the first time, to probe the warm dense matter regime

Astrophysical and weapons-related studies come directly into the area of warm dense matter

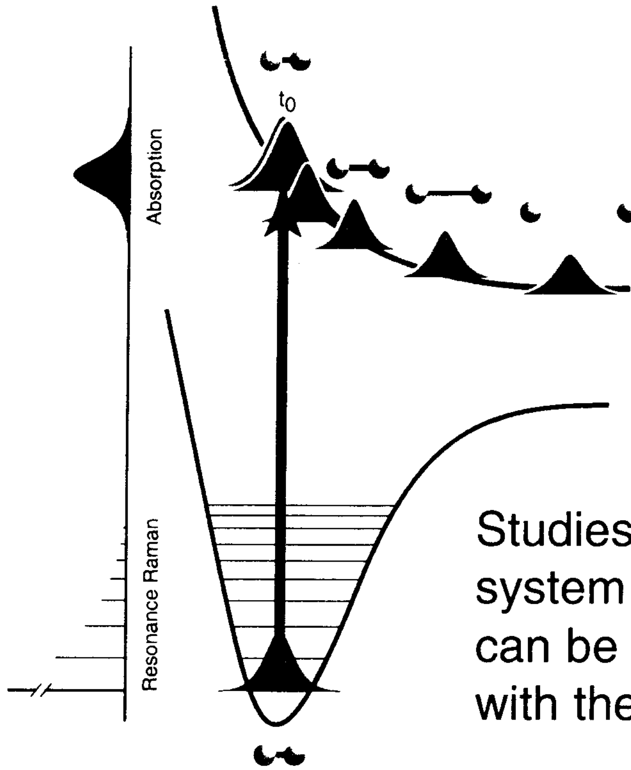
Regions of largest errors and uncertainties in many applied research areas of chemistry and physics come in the warm dense regime

Studies of Warm Dense Matter

•Use LCLS to create warm dense matter state and also (via delayed pulse) to probe it using x-ray scattering or imaging

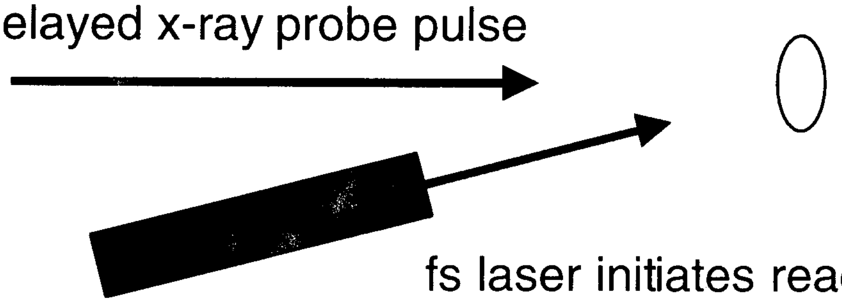
•Use conventional laser to selectively excite certain atomic transitions, creating population inversion which leads to lasing or plasma formation. Study the kinetics of this process using LCLS as probe

Femtosecond Chemistry



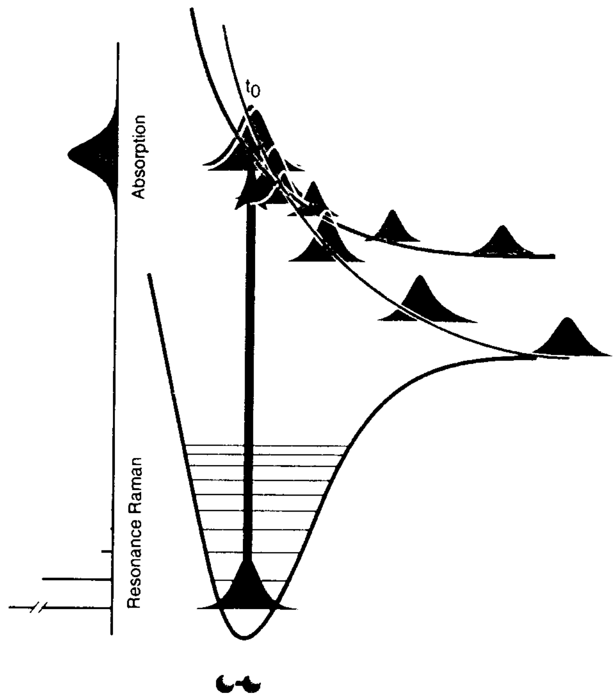
Studies of small system reactions can be compared with theory

Combine single-pulse x-ray diffraction with fast laser excitation



Femtosecond Chemistry

More realistic diatomic system



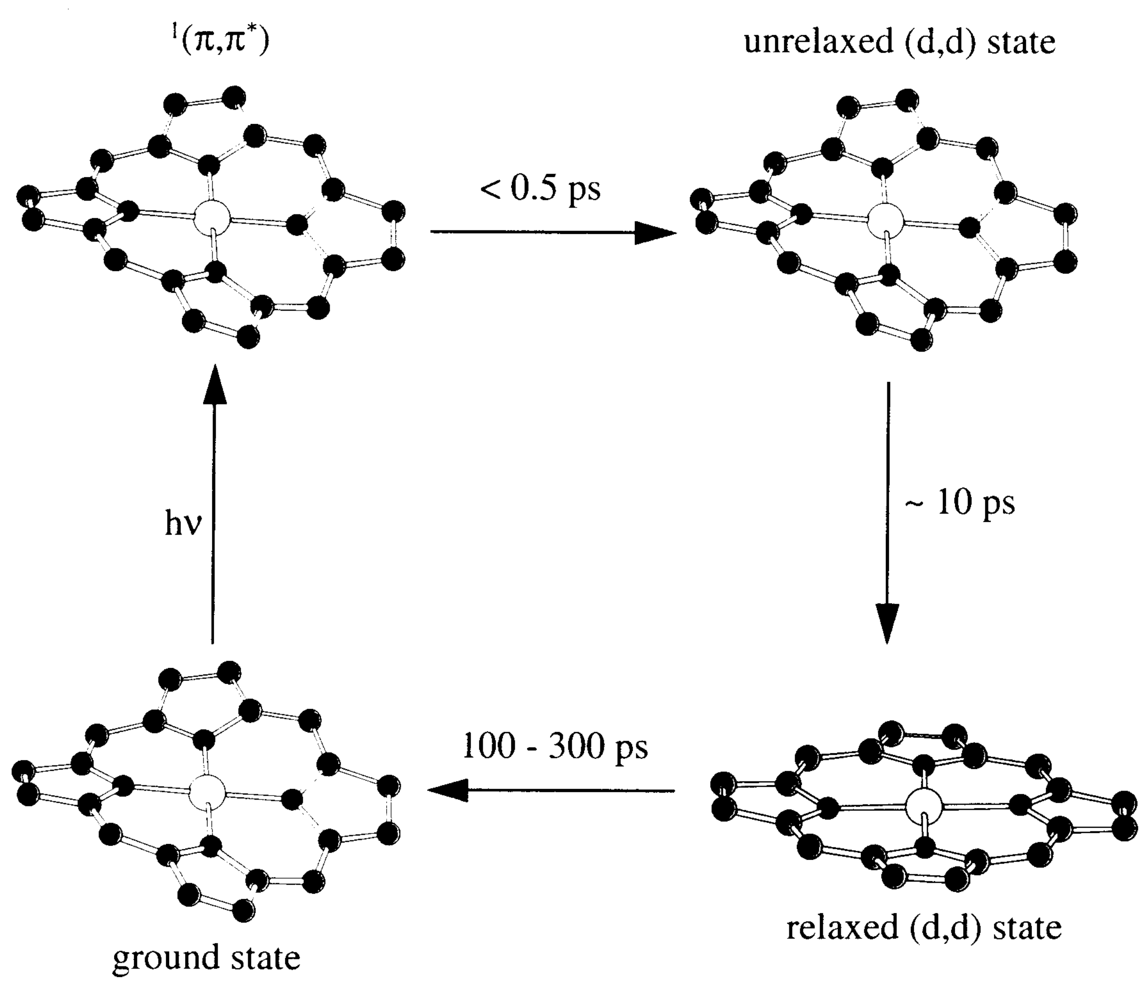
Photodissociation including surface hopping

Initial wavepacket prepared on the optically active red excited state, which is crossed by the dark gray state

As the wavepacket moves to near the crossing point a fraction of its amplitude crosses to the gray state, changing its electronic character in the process

Femtosecond Chemistry

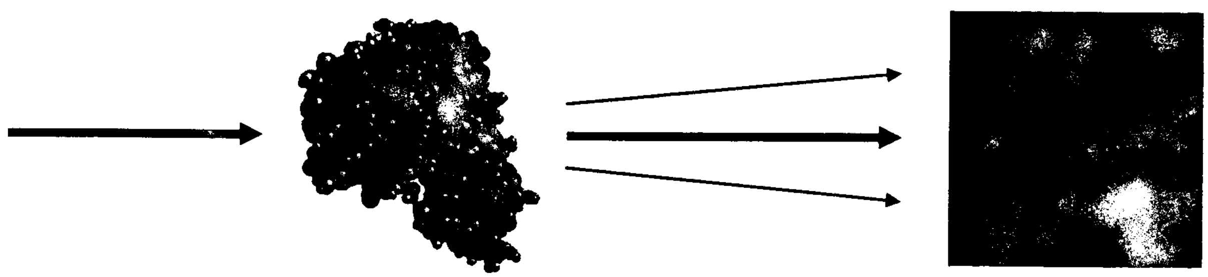
Goal: to study the sequence of structural changes that occur on a sub-ps time scale following an impulse trigger (laser-initiated reaction)



Low-spin (d^8) Nickel(II) Porphyrins deactivation pathway

X-Ray Diffraction from a Single Protein Molecule

Diffuse x-ray scattering from single protein molecule can be used to solve the protein structure



Lysozyme

Calculated scattering pattern from single lysozyme molecule

For 2Å resolution, need 10^{14} photons on protein
-> 10^{10} photons/Å^2, radiation dose ~ 10^{15} Gy

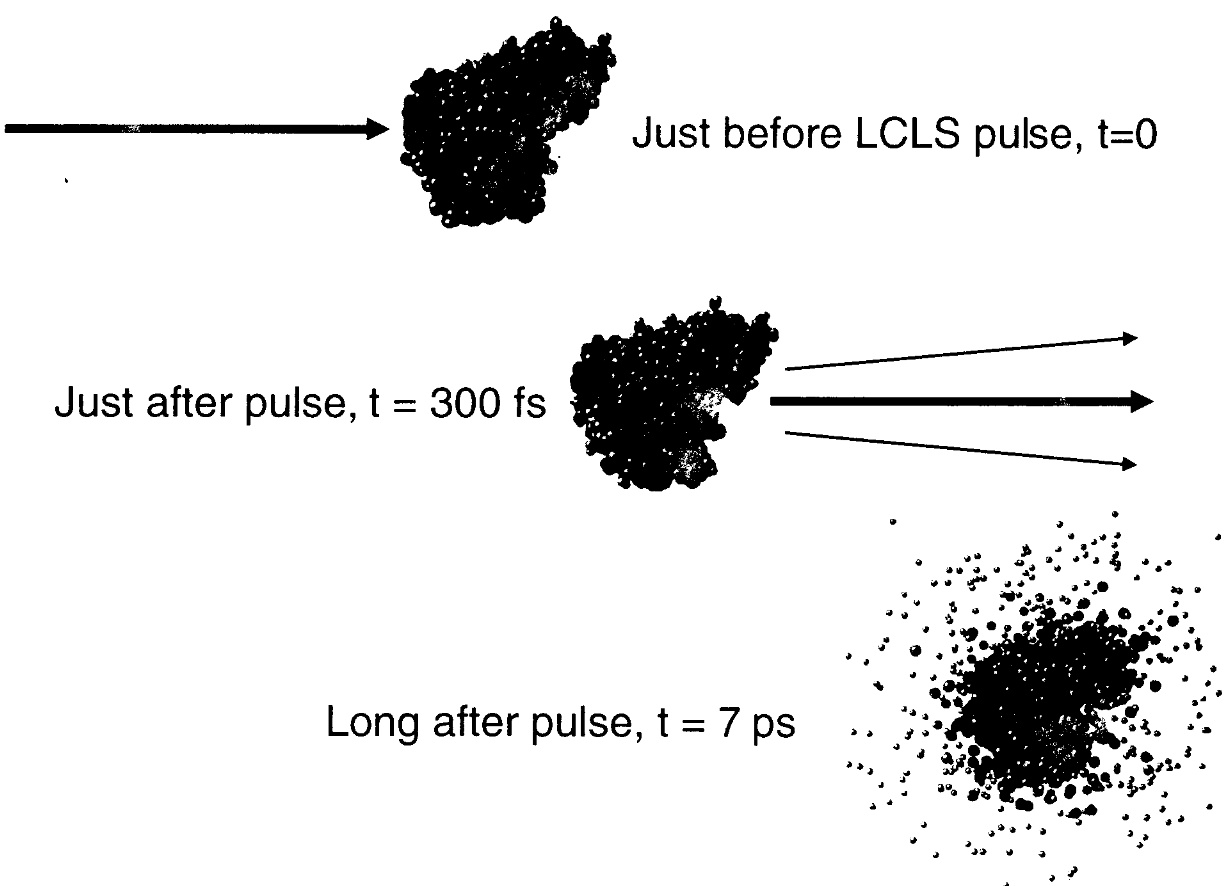
At 3rd gen. synchrotron source, 10^5 Gy destroys sample
10^7 Gy pulse will cause the sample to explode (~1 eV/atom)

X-Ray Diffraction from a Single Protein Molecule

A bright idea: A very short, intense x-ray pulse could produce a diffraction pattern before the molecule explodes

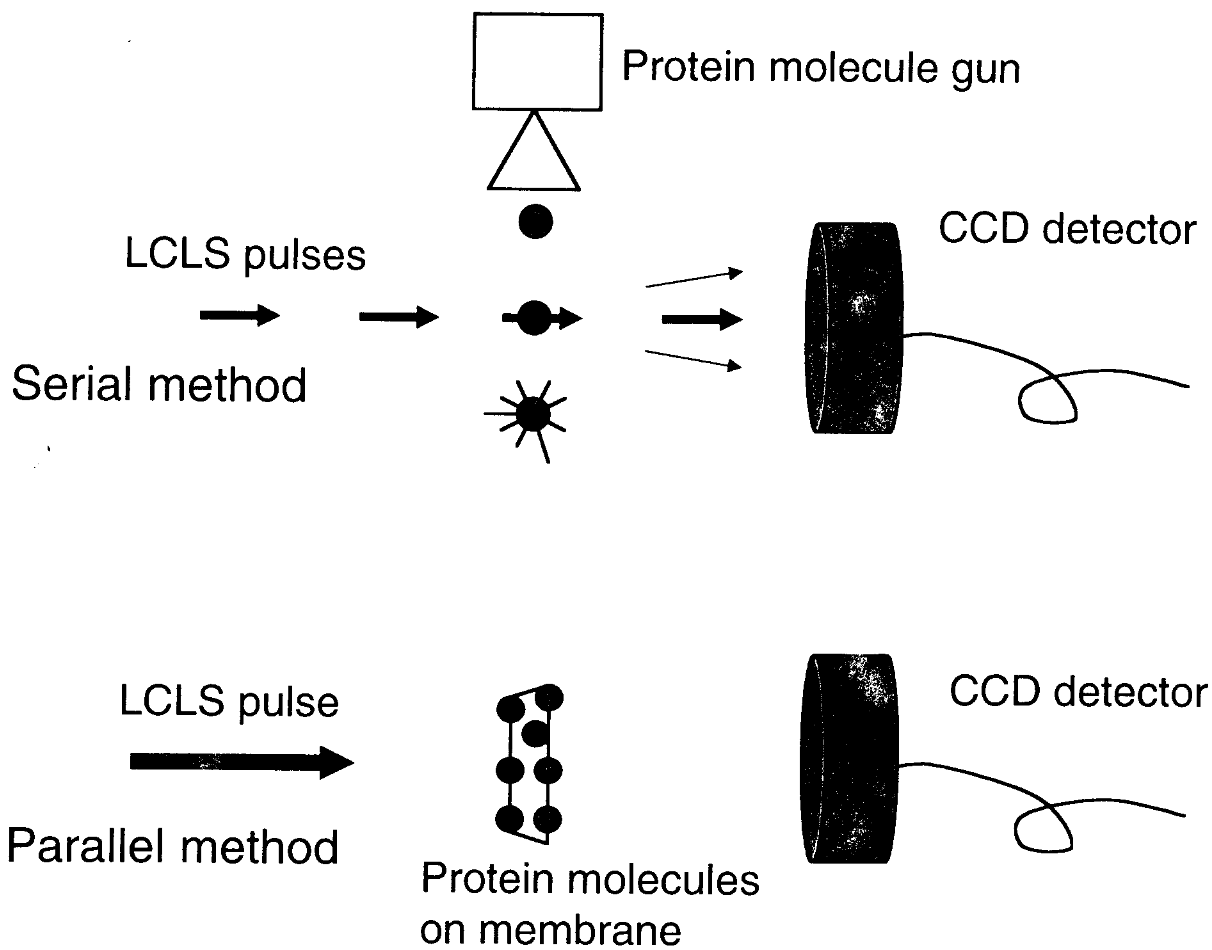
Janos Hajdu (Uppsala Univ.) and collaborators have used molecular dynamics calculations to study this idea. An important result:

- Lysozyme would survive LCLS pulse intensity for much longer than the 300 fs pulse length.



X-Ray Diffraction from a Single Protein Molecule

Complete 2Å structure would require multiple samples, orientations

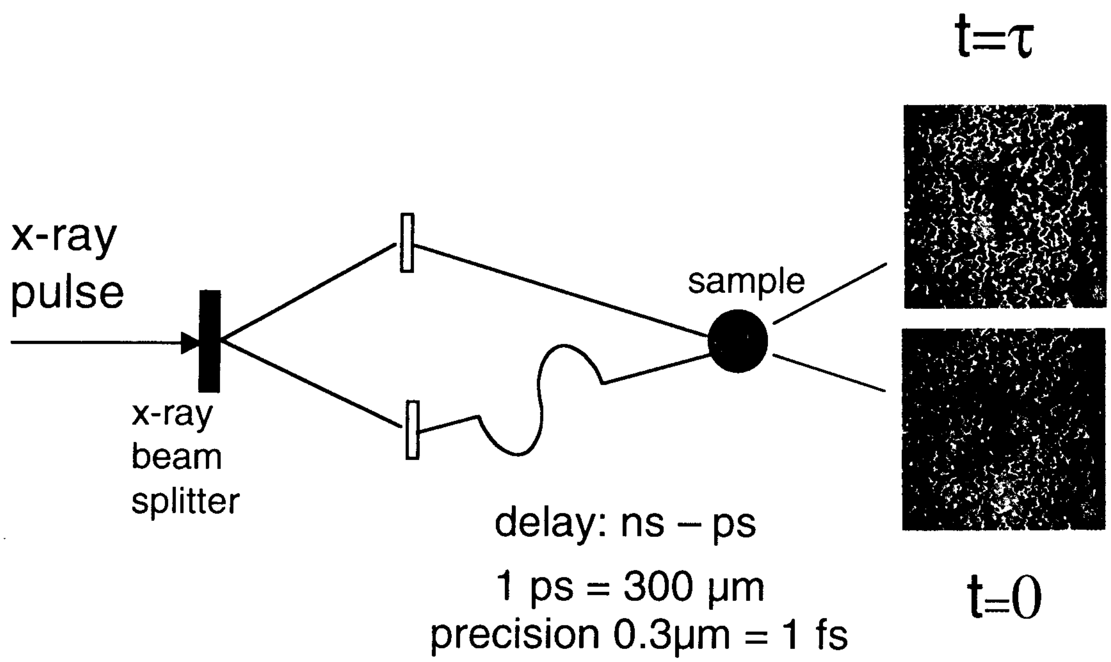


Nanoscale Dynamics in Condensed Matter

Study fast, atomic-scale motions in condensed systems using FEL pulse in various roles:

•X-ray probe followed by delayed x-ray probe studies equilibrium fluctuations

•X-ray or optical laser pump followed by x-ray probe studies relaxation dynamics



Nanoscale Dynamics in Condensed Matter

Possible areas of study

Simple Liquids – Transition from hydrodynamic to kinetic regime.
Complex Liquids – Effect of local structure on collective dynamics.
Polymers – Entanglement and reptation dynamics.
Glasses – Vibrational and relaxational modes in mesoscopic space-time region.
Dynamic Critical Phenomena – Order fluctuations in alloys, liquid crystals, etc.
Charge Density Waves – Direct observation of sliding dynamics.
Quasicrystals – Nature of phason and phonon dynamics.
Surfaces – Dynamics of adatoms, islands, and steps during growth and etching.
Defects in Crystals – Diffusion, dislocation glide, domain dynamics.
Ferroelectrics – Order-disorder vs. displacive nature; anisotropic correlations and size effects.

Single-Shot Science

Detector must simultaneously record positions or angles of about 10^{12} photons

Atomic physics
FEL beam excites atoms into novel states
Direct observation of multiple core hole formation (MCHF) or multiphoton ionization of a K-shell electron (MPIK), giant coulomb explosions in atomic cluster (GCEC)

Biology
Scattering patterns from very small crystals or molecular clusters
Atomic structures of proteins that do not form large crystals

Condensed matter physics and materials science
Speckle patterns

Fast Time-Resolved Science

Time resolution in the femtosecond to nanosecond range required, through fast detector or well-synchronized pump-probe

Atomic physics
Relaxation of novel atomic states

Warm dense matter physics
Relaxation of warm dense matter state
Deduce equation of state of matter in this regime; implications for astrophysics, explosion physics

Femtosecond chemistry
Time evolution of chemical reactions
Study the sequence of structural changes that occur on a sub-ps time scale following an impulse trigger (laser-initiated reaction)

Condensed matter physics and materials science
Photon correlation spectroscopy
Dynamics of simple liquids, complex liquids, polymers, glasses, critical phenomena, charge density waves, quasicrystals, surfaces, crystal defects, ferroelectrics

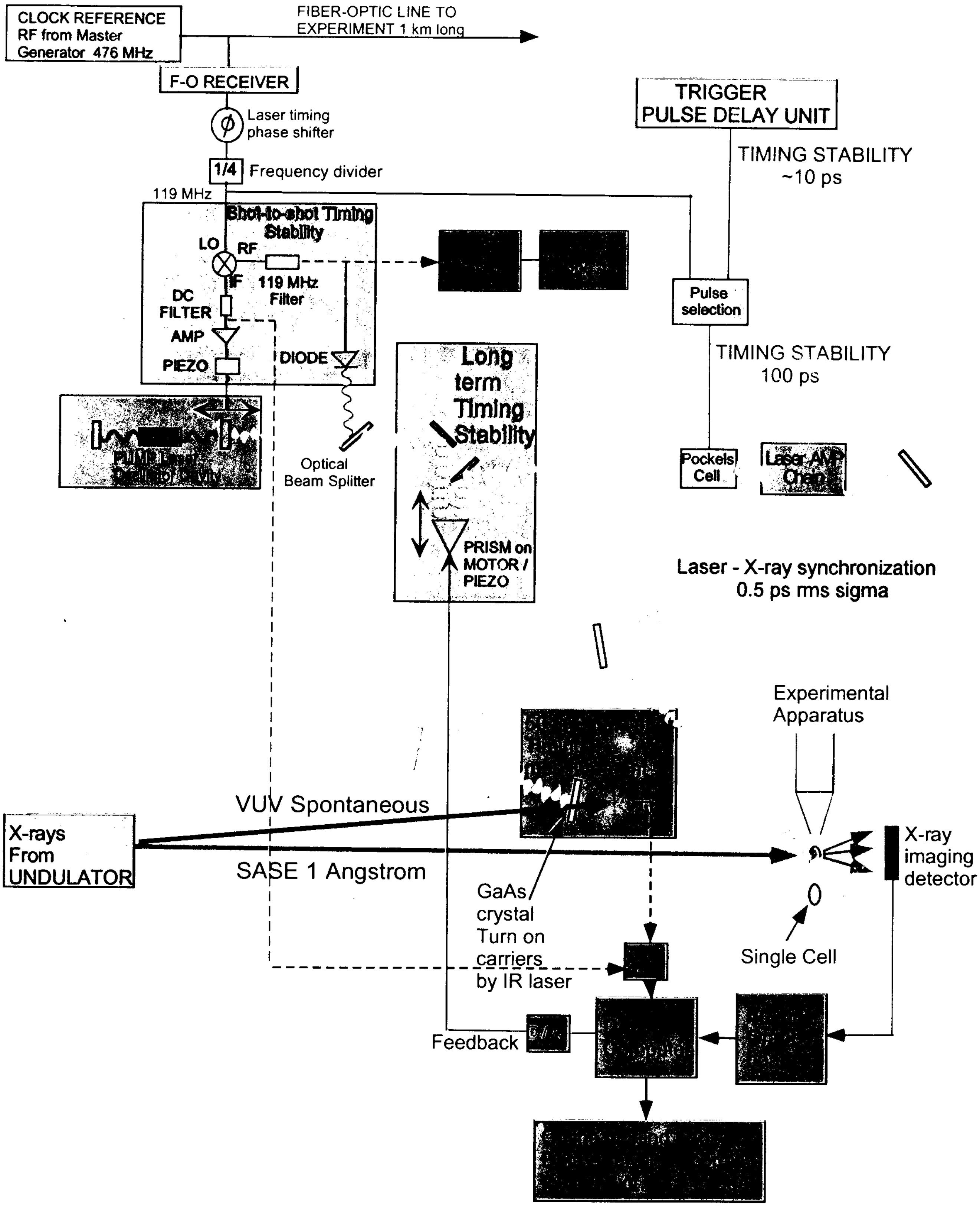
A possible fast timing strategy

For pump-probe experiments using FEL x-ray pulse and external laser:

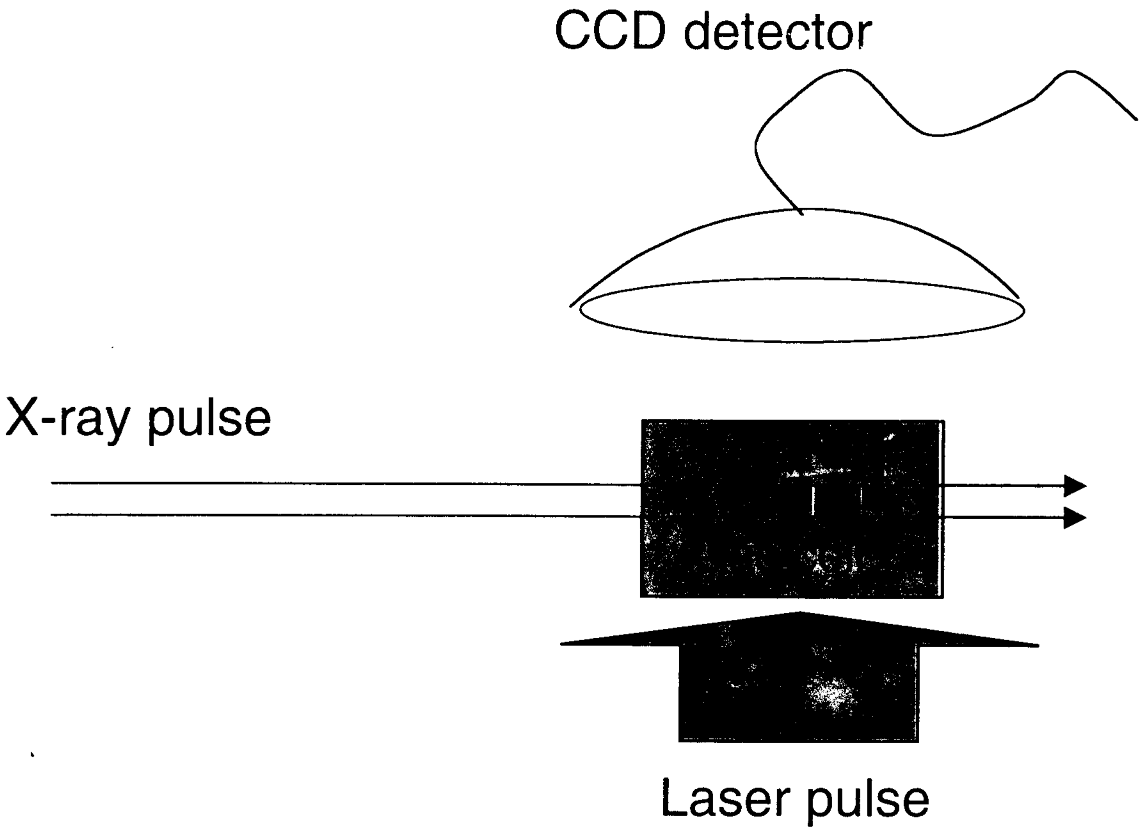
1) Do the best job possible of reducing timing jitter between FEL and laser (expect jitter ~ 0.5 ps)

2) Use accurate correlation measurement and data binning for shorter pump-probe delays (hope for correlation measurement accuracy ~ 50 fs)

LCLS EXPERIMENTAL ROOM
PUMP-PROBE SYNCHRONIZED AT 0.5 ps
BUT DATA BINNING AT 50 fs TIMING RESOLUTION



Sub-ps correlation of laser and x-ray pulses



X-ray pulse excites gas atoms, changes transmission for laser pulse

Large crossing angle and large laser beam size convert time into distance

9 mm ~ 30 ps

Conclusions

X-ray free-electron lasers have the potential to facilitate exciting new science in several disciplines.

In order to reach this potential, detector development is required.

•Some experiments require a detector which can measure the positions of about 10^{12} photons which arrive almost simultaneously

•Some experiments require a detector system which can determine the coincidence of an x-ray and a laser pulse with femtosecond accuracy